SG39 Meeting
November 20-21, 2017

Update on Continuous Energy Cross Section Adjustment.

UC Berkeley / INL collaboration

Outline

- Brief recall of the continuous-energy adjustment methodology
- eXtended Generalized Perturbation Theory (xGPT) in Serpent
- Releted Monte Carlo methods

Continuous-energy first order uncertainty propagation

$$Var\left[R\right] = \int_{E_{min}}^{E_{max}} \int_{E_{min}}^{E_{max}} S_{\Sigma}^{R}\left(E\right) \cdot COV\left[\Sigma(E)\,,\Sigma(E')\right] \cdot S_{\Sigma}^{R}\left(E'\right)\, dE\, dE' \tag{1}$$

$COV\left[\Sigma(E)\,,\Sigma(E')\right]$ is the continuous-energy covariance matrix

$S_{\Sigma}^{R}\left(E\right)$ is the sensitivity density function for the generic response R

Multi-group discretization is usually introduced here

Multi-group discretization of the covariance matrix

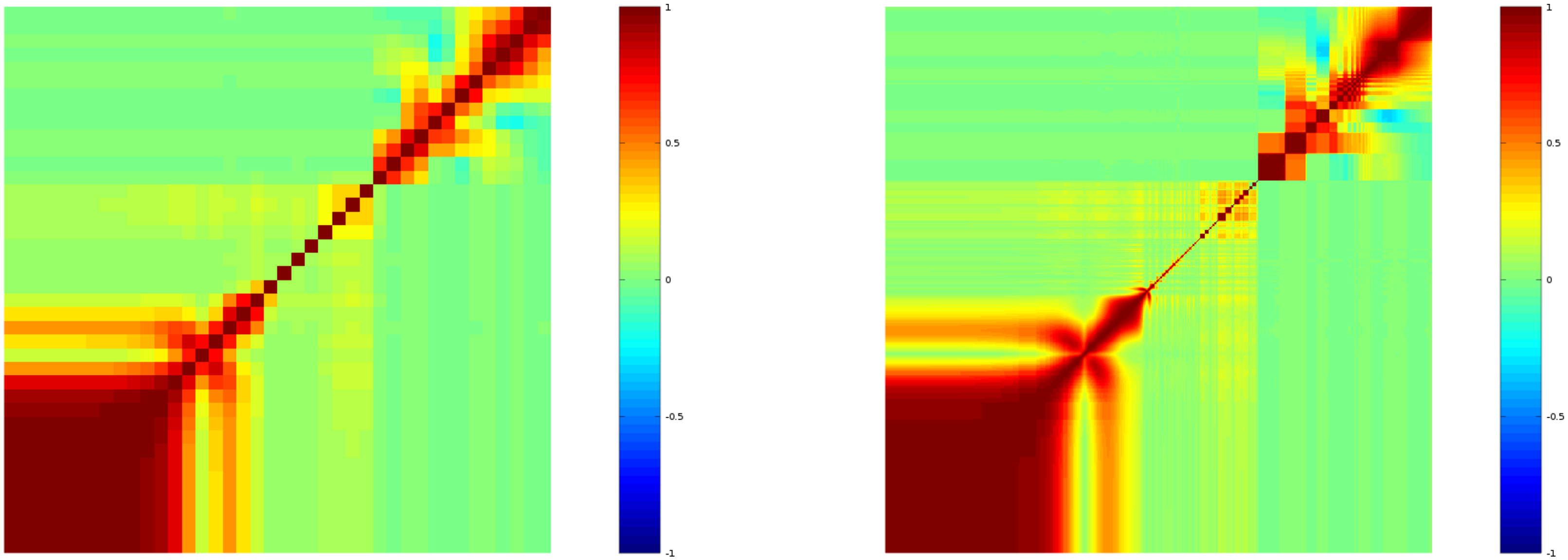

Figure: Comparison between the multi-group (left) and continuous (right) ^{239}Pu capture cross correlation matrices adopted in the adjustment process.

Multi-group discretization of the covariance matrix

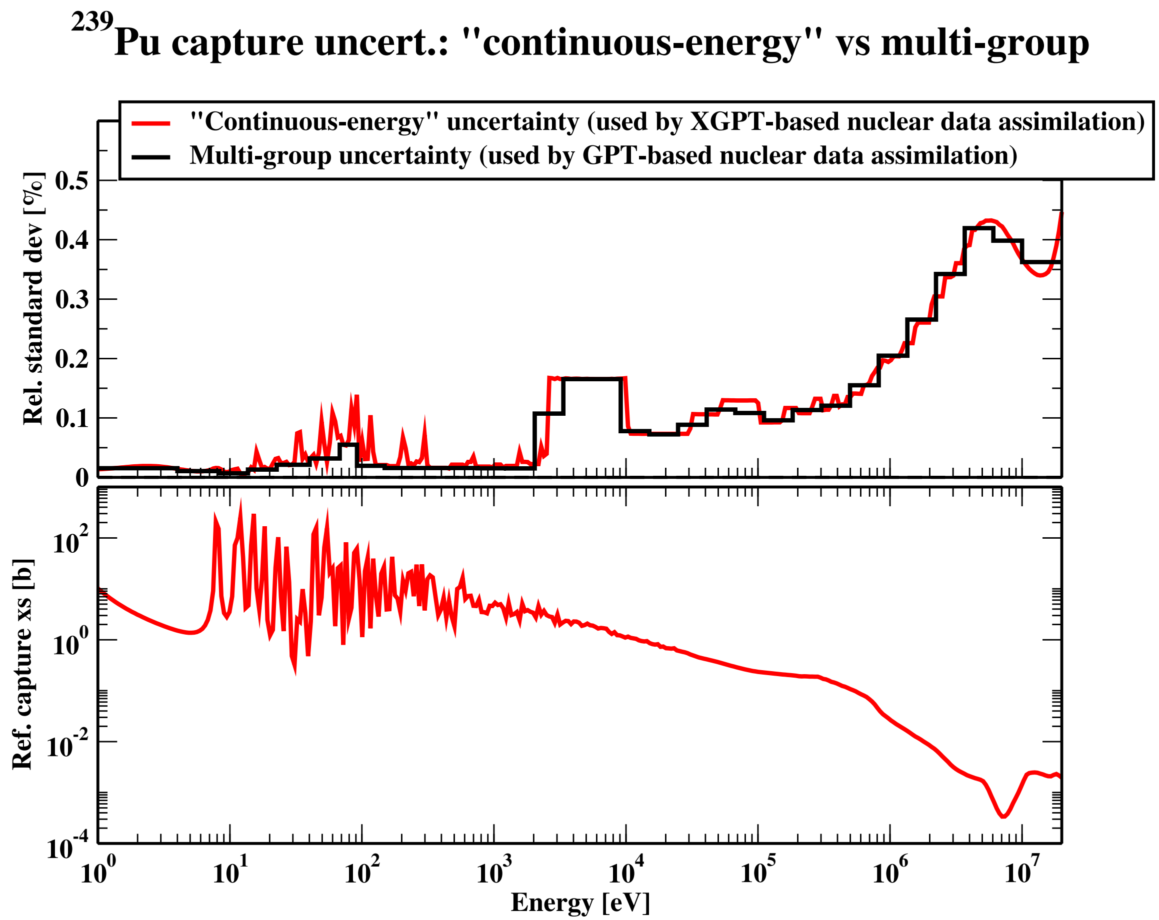

Figure: Comparison between ^{239}Pu capture cross section relative uncertainty adopted as input by the "continuous" and multi-group approaches.

Eigendecomposition of the covariance matrix

$$COV\left[\Sigma(E)\,,\Sigma(E')\right] = \sum_{j=1}^{\infty} U_j(E)\cdot V_j \cdot U_j(E') \quad (2)$$

V_j are the eigenvalues of the continuous energy covariance matrix corresponding to the eigenfunctions $U_j(E)$

Continuous-energy uncertainty propagation (revisited)

$$Var\left[R\right] = \int\limits_{E_{min}}^{E_{max}} \int\limits_{E_{min}}^{E_{max}} S_{\Sigma}^{R}\left(E\right) \cdot COV\left[\Sigma(E)\,, \Sigma(E')\right] \cdot S_{\Sigma}^{R}\left(E'\right)\, dE\, dE' \tag{1}$$

$$Var\left[R\right] = \sum_{j=1}^{\infty} V_j \cdot \left(\int\limits_{E_{min}}^{E_{max}} U_j\left(E\right) \cdot S_{\Sigma}^{R}\left(E\right)\, dE \right)^2 \tag{3}$$

Continuous-energy uncertainty propagation (revisited)

$$Var\left[R\right] = \int\limits_{E_{min}}^{E_{max}} \int\limits_{E_{min}}^{E_{max}} S_{\Sigma}^{R}\left(E\right) \cdot COV\left[\Sigma(E)\,,\Sigma(E')\right] \cdot S_{\Sigma}^{R}\left(E'\right)\, dE\, dE' \tag{1}$$

$$Var\left[R\right] = \sum_{j=1}^{\infty} V_j \cdot \left(S_{U_j}^{R}\right)^2 \simeq \sum_{j=1}^{n} V_j \cdot \left(S_{U_j}^{R}\right)^2 \tag{3}$$

Continuous energy cross section adjustment

Adjustment parameters $\boldsymbol{\Delta}_{\boldsymbol{U}} = [\Delta_{U_1}, \Delta_{U_2} \cdots \Delta_{U_n}]^T$:

$$\boldsymbol{\Delta}_{\boldsymbol{U}} = \mathbf{M}\,\mathbf{G}^T \left[\mathbf{G}\,\mathbf{M}\,\mathbf{G}^T + \mathbf{V_e} + \mathbf{V_m}\right]^{-1} \mathbf{D_R} \qquad (4)$$

- $\mathbf{M}$ is the prior covariance of the continuous functions ${}^{prior}\mathbf{COV}\,[\mathbf{U}\,,\mathbf{U}]$
- $\mathbf{V_e}$ and $\mathbf{V_m}$: matrices of the experimental and modeling errors
- $\mathbf{D_R}$ contains the relative differences between the calculated and measured experiments.
- $\mathbf{G}$ is the matrix of the sensitivities: $\mathbf{G} = \left[\mathbf{S}_{\mathbf{U}}^{\mathbf{R}_1}\mathbf{S}_{\mathbf{U}}^{\mathbf{R}_2} \cdots \mathbf{S}_{\mathbf{U}}^{\mathbf{R}_N}\right]^T$

Continuous energy cross section adjustment

$$\mathbf{\Delta}_U = \mathbf{M}\,\mathbf{G}^T\left[\mathbf{G}\,\mathbf{M}\,\mathbf{G}^T + \mathbf{V_e} + \mathbf{V_m}\right]^{-1}\,\mathbf{D_R} \tag{4}$$

$$^{adjusted}\Sigma\left(E\right) \simeq {}^{prior}\Sigma\left(E\right)\cdot\left(1 + \sum_{j=1}^{n}\Delta_{U_j}\cdot U_j\left(E\right)\right) \tag{5}$$

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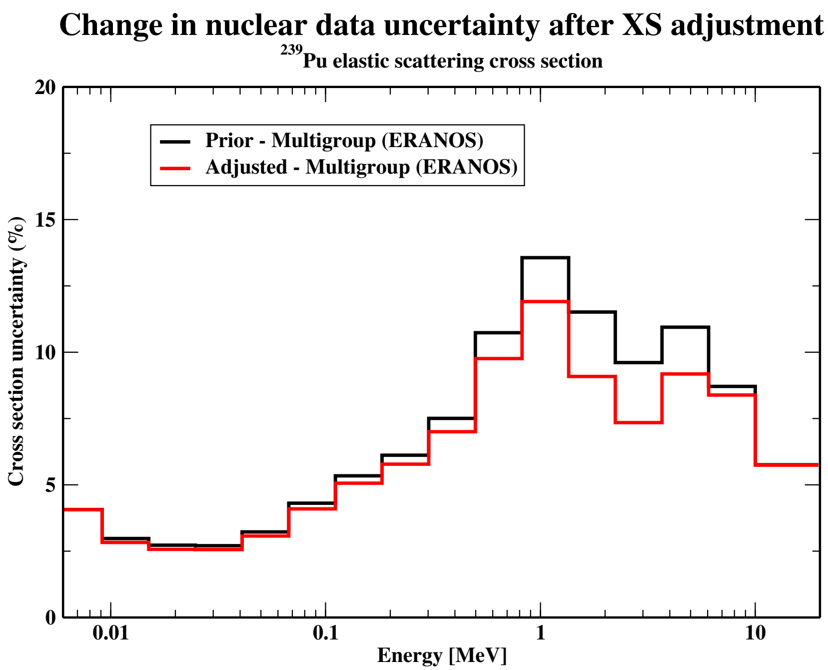
	Prior rel. uncert. (%)		Post rel. uncert. (%)	
	multi-group	XGPT	multi-group	XGPT
k_{eff}	0.733	0.704	0.191	0.190
F28/F25	3.731	3.581	1.298	1.291
F37/F25	3.631	3.573	1.307	1.306
F49/F25	0.825	0.797	0.558	0.547

Table: Comparison of prior (input) and post (adjusted) nuclear data uncertainties estimated by the multi-group and continuous approaches for the four response functions.



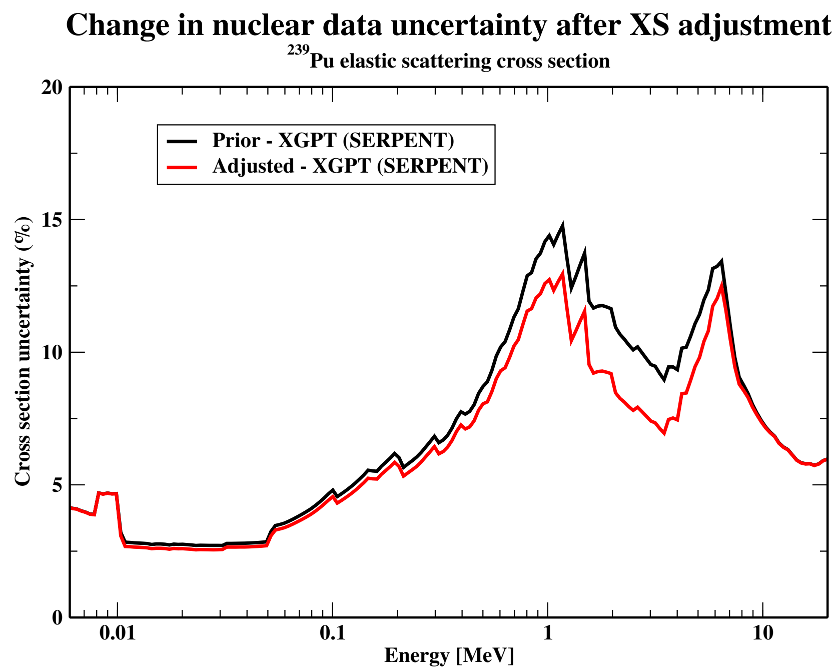
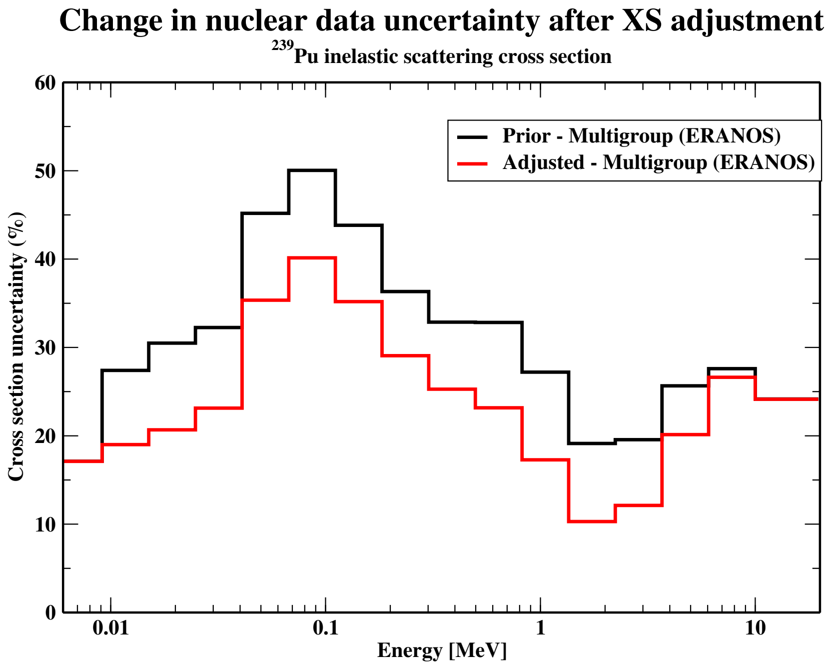


Figure: ^{239}Pu elastic scattering uncertainty before and after the adjustment process. Multi-group (left) and continuous energy (right) results.

Continuous vs. multi-group: uncertainty reduction
Jezebel–^{239}Pu Case study



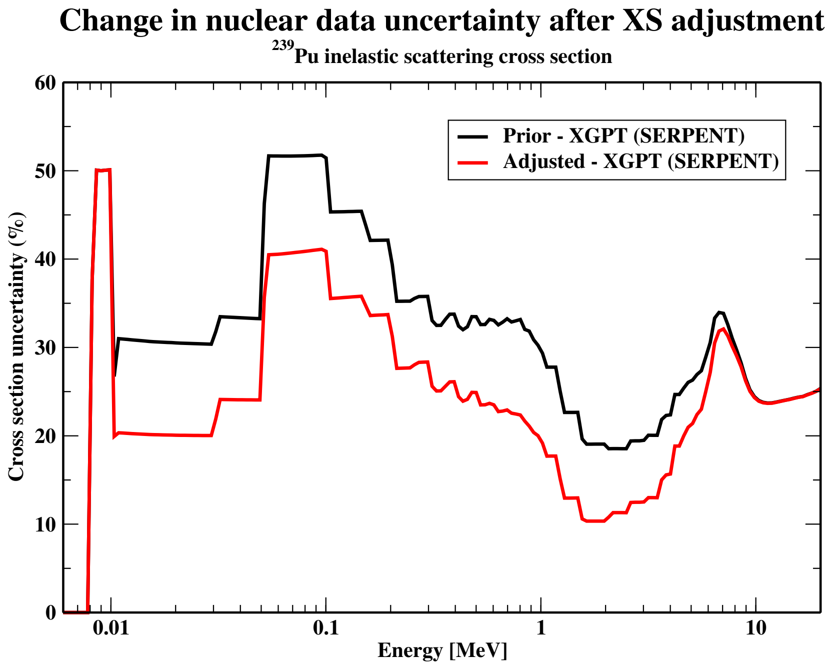


Figure: ^{239}Pu inelastic scattering uncertainty before and after the adjustment process. Multi-group (left) and continuous energy (right) results.

Continuous vs. multi-group: XS adjustment
Jezebel–^{239}Pu Case study

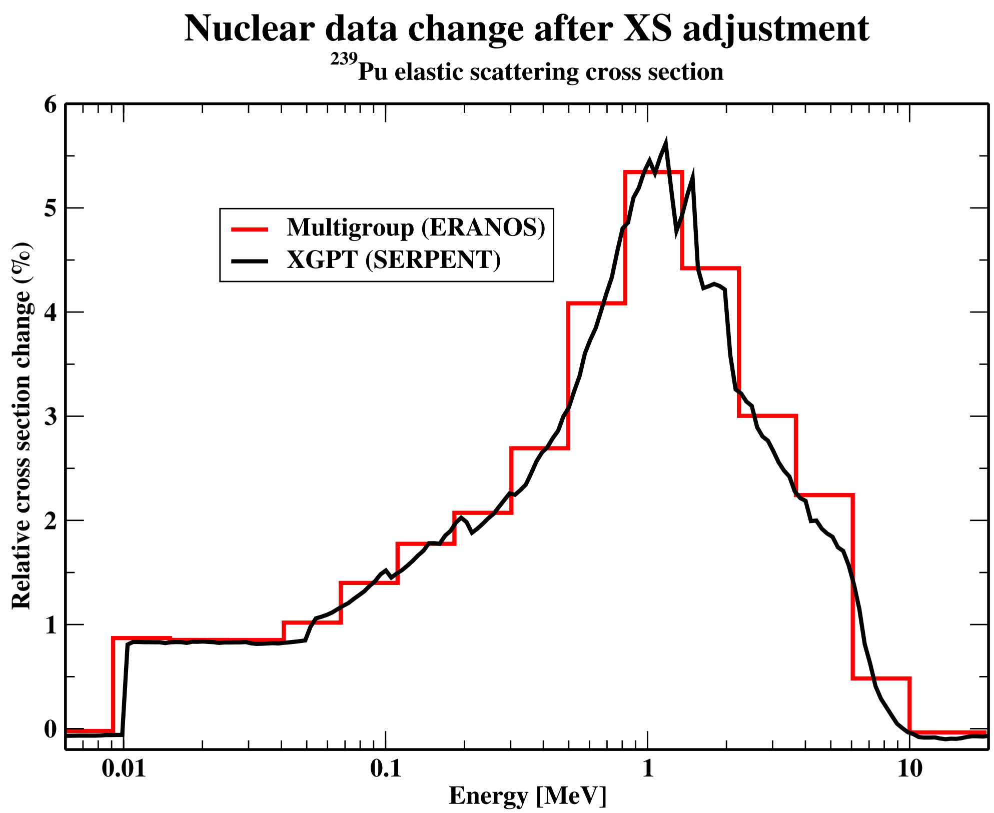


Figure: ^{239}Pu elastic scattering cross section before and after the adjustment process. Multi-group (red) and continuous energy (black) results.

Continuous vs. multi-group: XS adjustment
Jezebel–^{239}Pu Case study

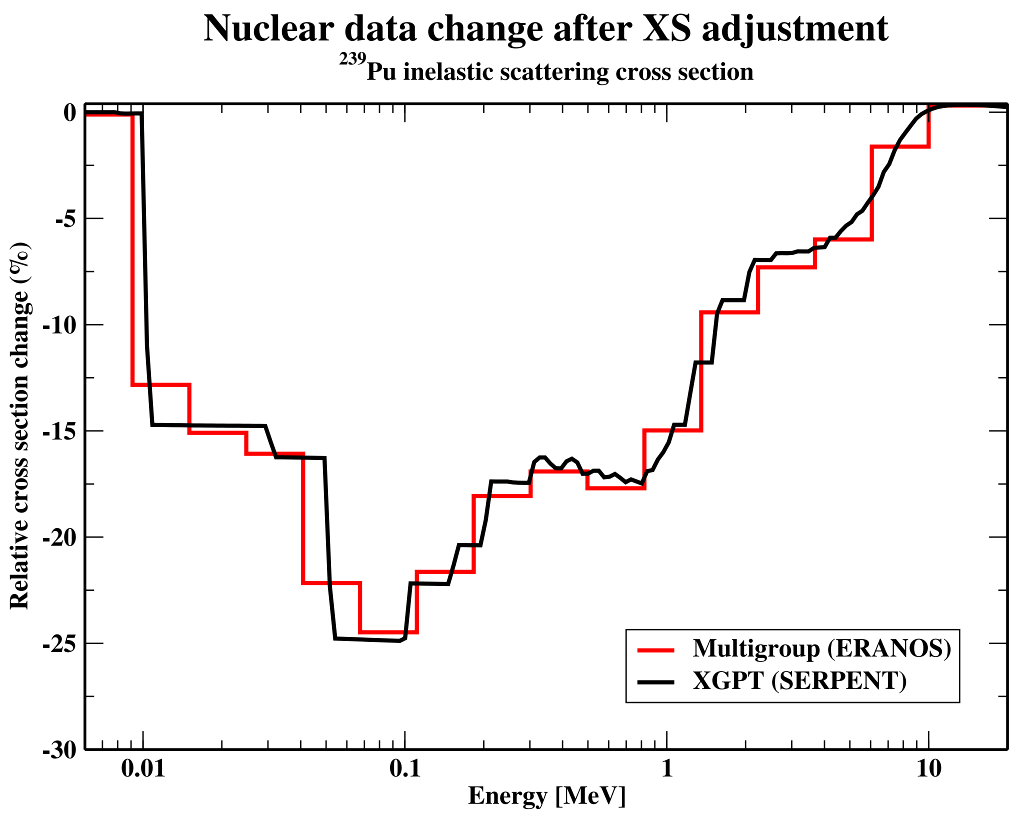


Figure: ^{239}Pu inelastic scattering cross section before and after the adjustment process. Multi-group (red) and continuous energy (black) results.

Continuous vs. multi-group: Post C/E

Jezebel–^{239}Pu Case study

	Prior C/E		Post C/E	
	multi-group [1]	XGPT	multi-group	XGPT
k_{eff}	0.99986	0.99976	1.00001	1.00000
F28/F25	0.977	0.979	0.995	0.995
F37/F25	0.987	0.988	0.996	0.996
F49/F25	0.975	0.975	0.985	0.984

Table: Comparison of prior and post C/E estimated by the multi-group and continuous approaches for the four response functions.

xGPT is now available in Serpent 2.1.19 (minor limitations will be fixed)

Most of the continuous-energy sensitivity capabilities required for the adjustment methodology are now available to all Serpent users thanks to Ville's xGPT implementation in the official release.

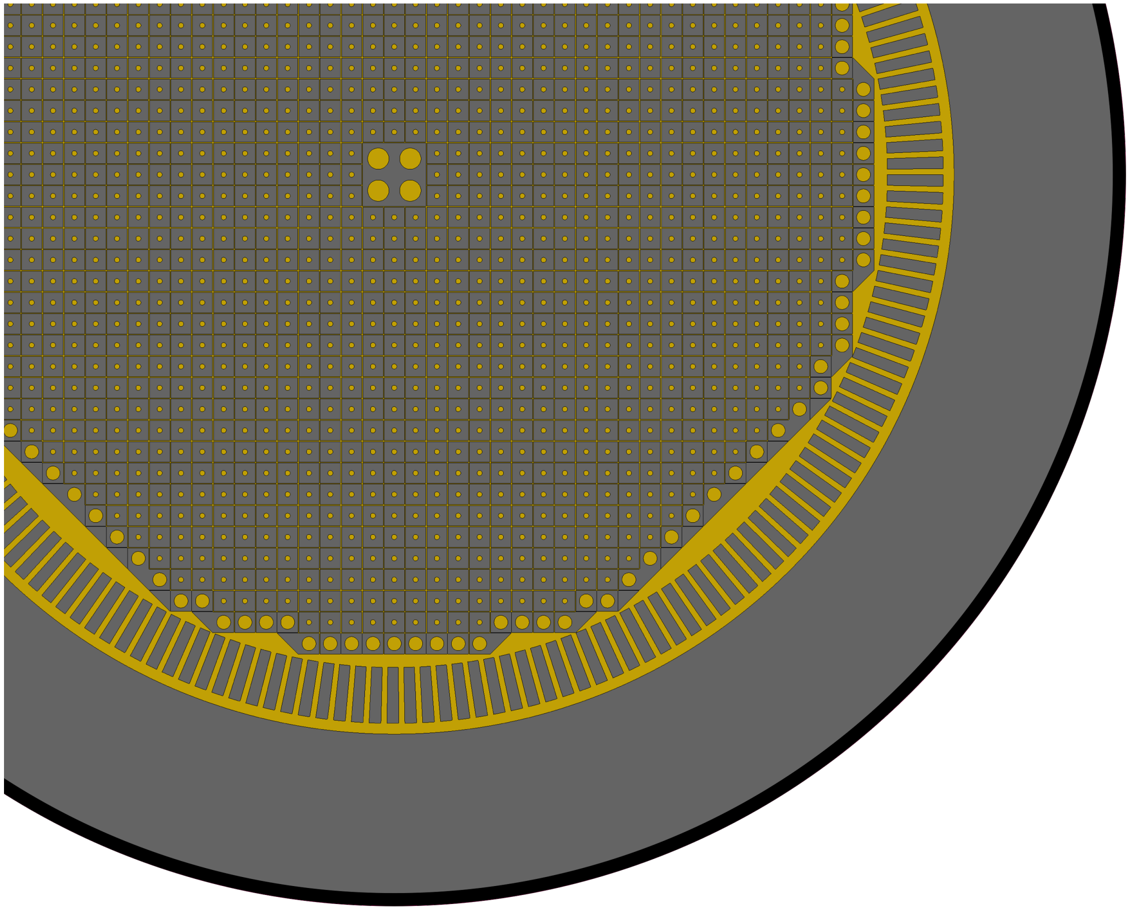
Info on the sensitivity capabilities made avaialble in Serpent:
Ville.Valtavirta@vtt.fi

serpent.vtt.fi/mediawiki/index.php/Sensitivity_Calculations

serpent.vtt.fi/mediawiki/index.php/XGPT_example

Different applications of xGPT capabilities

^{233}U uncertainties in the Molten Salt Breeder Reactor



Sensitivity/uncertainty study for the ^{233}U resonance parameters in the Molten Salt Breeder Reactor. JENDL-4 ENDF File *MF-32*.

UC Berkeley student Michael Martin

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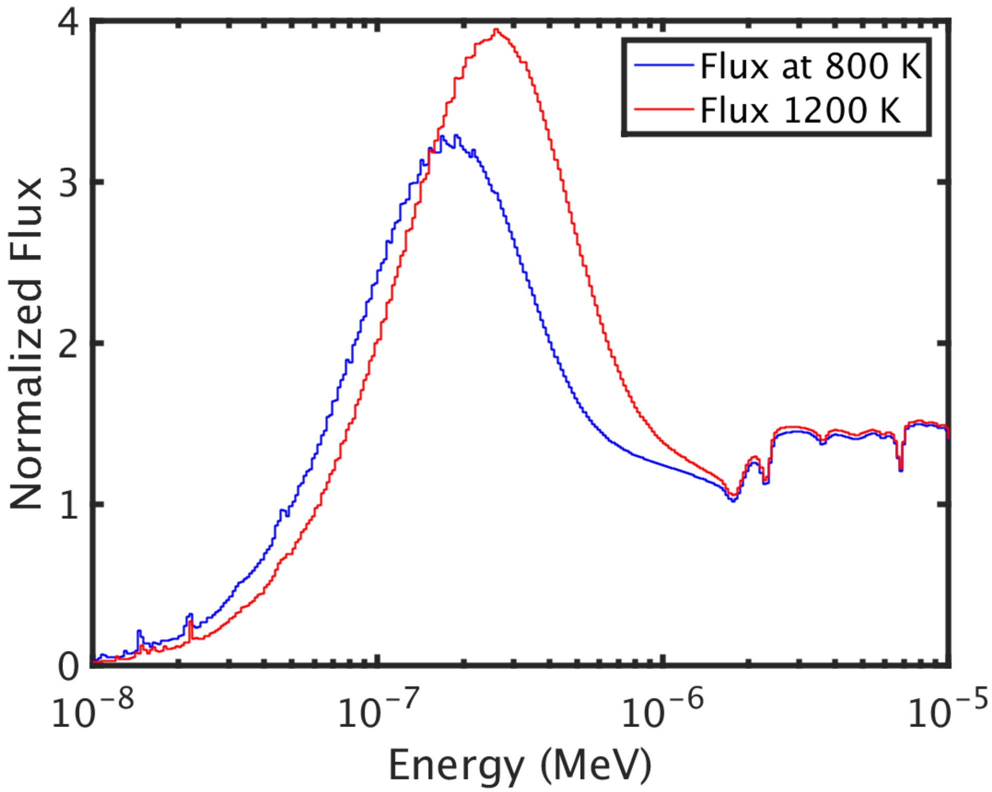
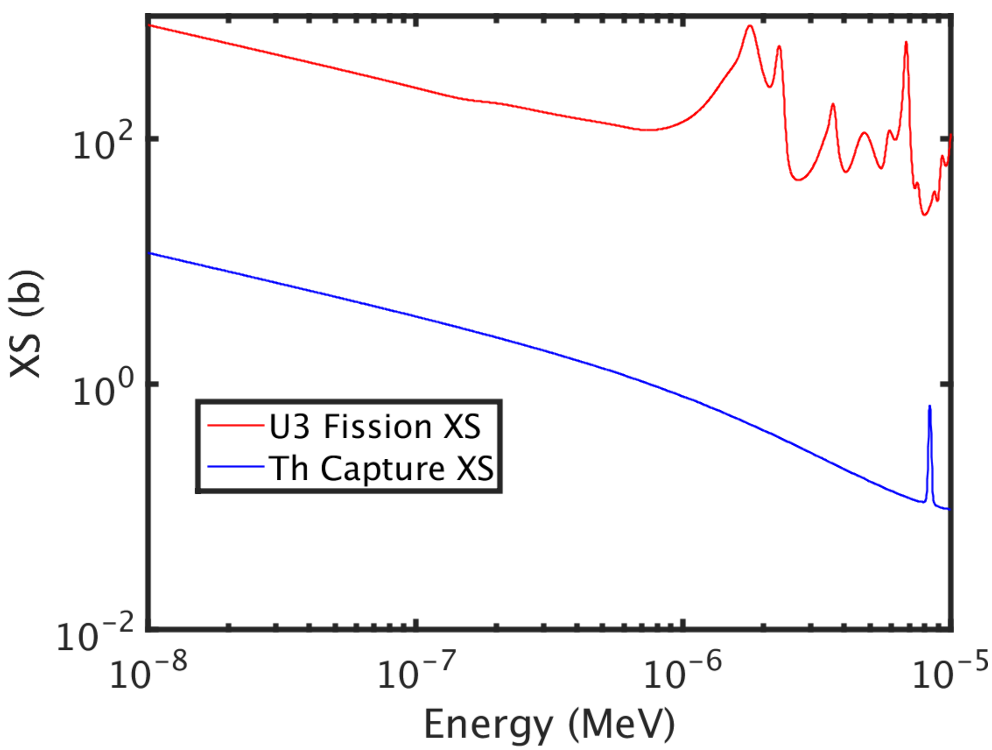
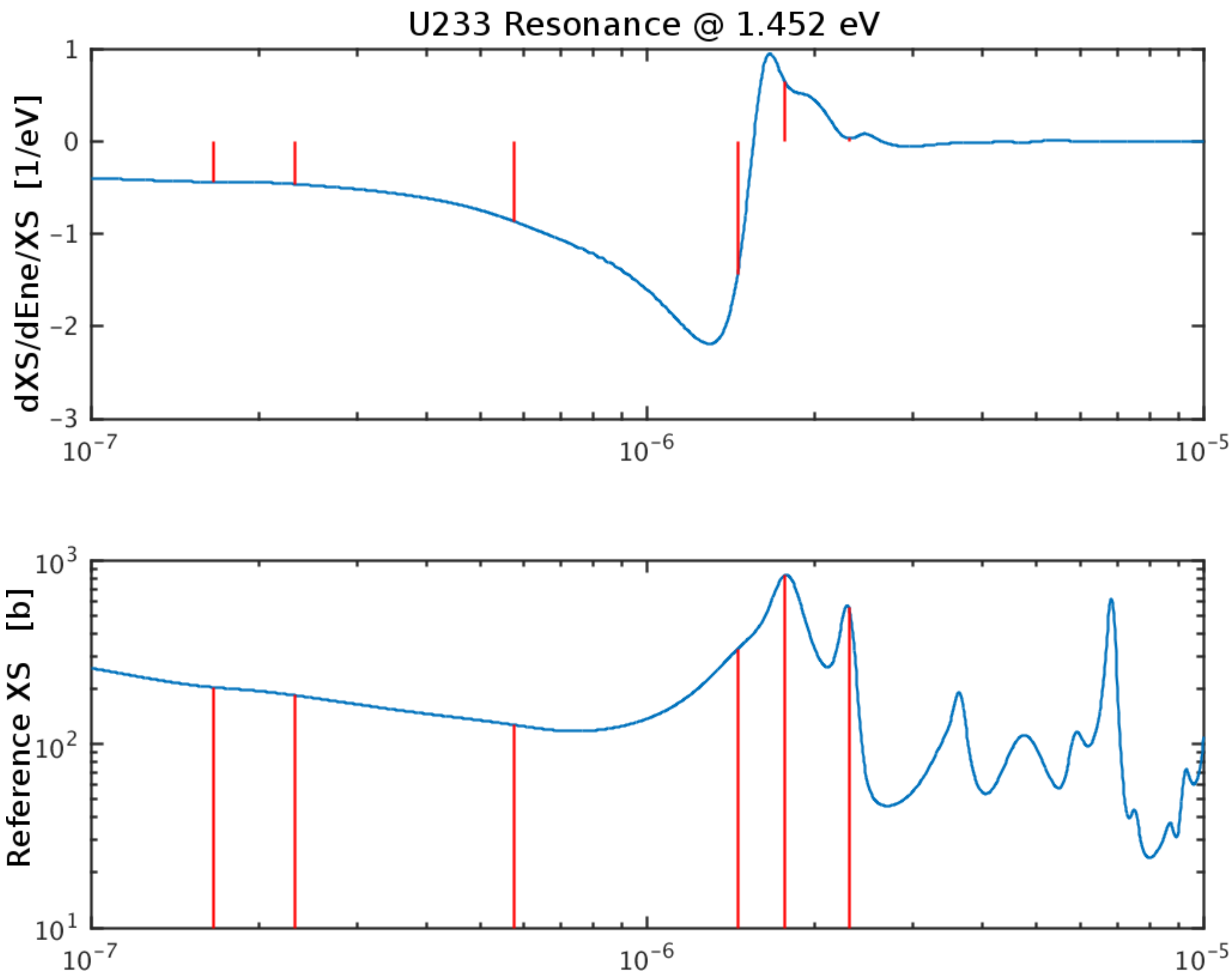
^{233}U uncertainties in the Molten Salt Breeder Reactor





Cross sections derivatives

^{233}U Fission cross section

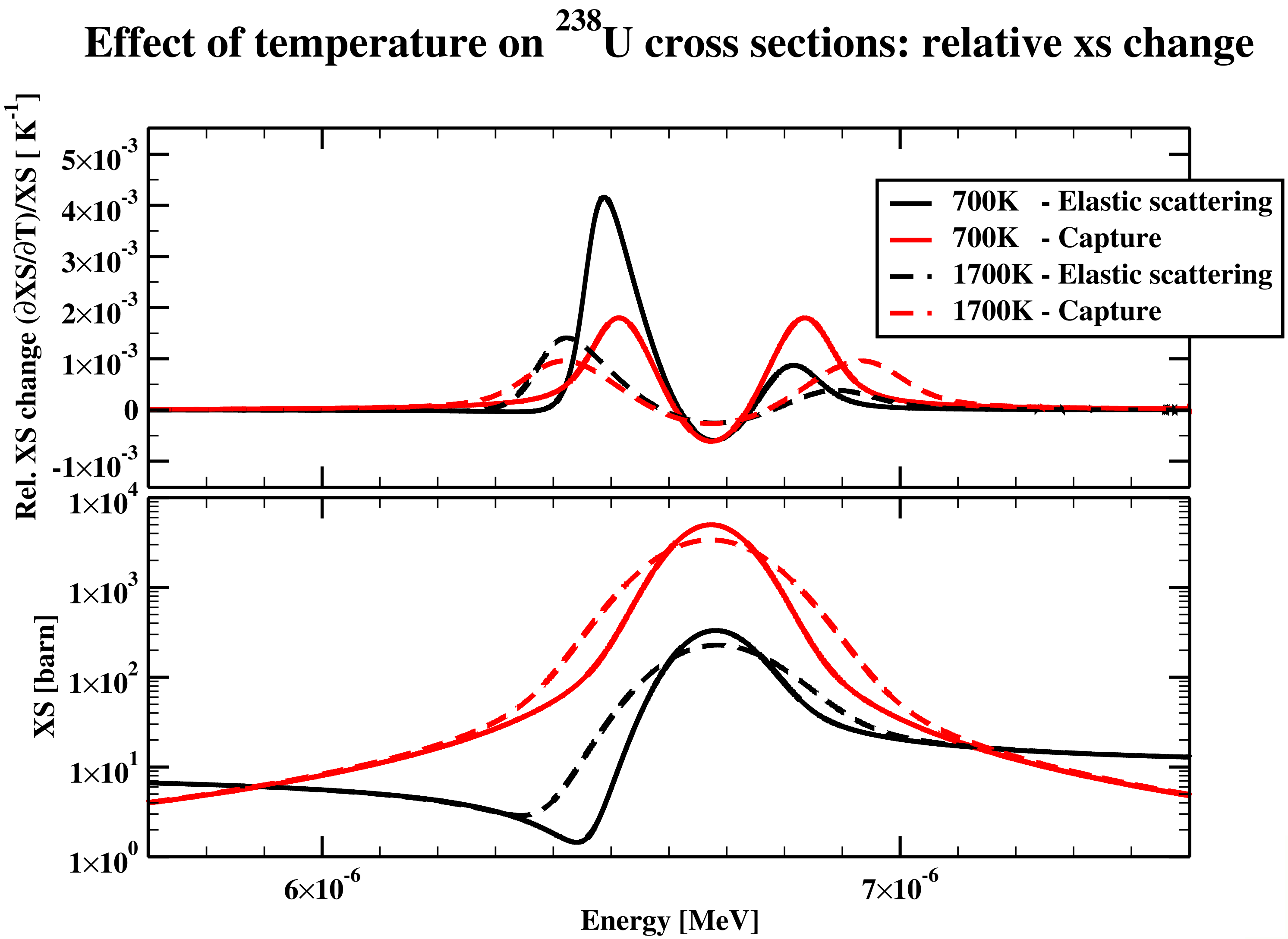


Verification against direct perturbation

Parameter	Reference (direct perturbation)	Perturbation Theory (XGPT)	Absolute Difference
Resonance at 1.452 eV			
$S_{E}^{k_{eff}}$ $[eV^{-1}]$	$-1.35 \cdot 10^{-1} \pm 5.0 \cdot 10^{-4}$	$-1.32 \cdot 10^{-1} \pm 6.1 \cdot 10^{-5}$	$3.63 \cdot 10^{-3}$
$S_{\Gamma_n}^{k_{eff}}$ [-]	$7.94 \cdot 10^{-2} \pm 1.4 \cdot 10^{-4}$	$8.09 \cdot 10^{-2} \pm 2.4 \cdot 10^{-5}$	$1.50 \cdot 10^{-3}$
$S_{\Gamma_\gamma}^{k_{eff}}$ [-]	$-9.40 \cdot 10^{-3} \pm 1.5 \cdot 10^{-4}$	$-9.34 \cdot 10^{-3} \pm 3.3 \cdot 10^{-6}$	$6.30 \cdot 10^{-5}$
$S_{\Gamma_{F_a}}^{k_{eff}}$ [-]	$9.80 \cdot 10^{-4} \pm 2.8 \cdot 10^{-5}$	$9.53 \cdot 10^{-4} \pm 2.6 \cdot 10^{-7}$	$2.71 \cdot 10^{-5}$

Direct perturbation verification by Michael Martin UC Berkeley

Doppler reactivity coeff. calculation via XGPT



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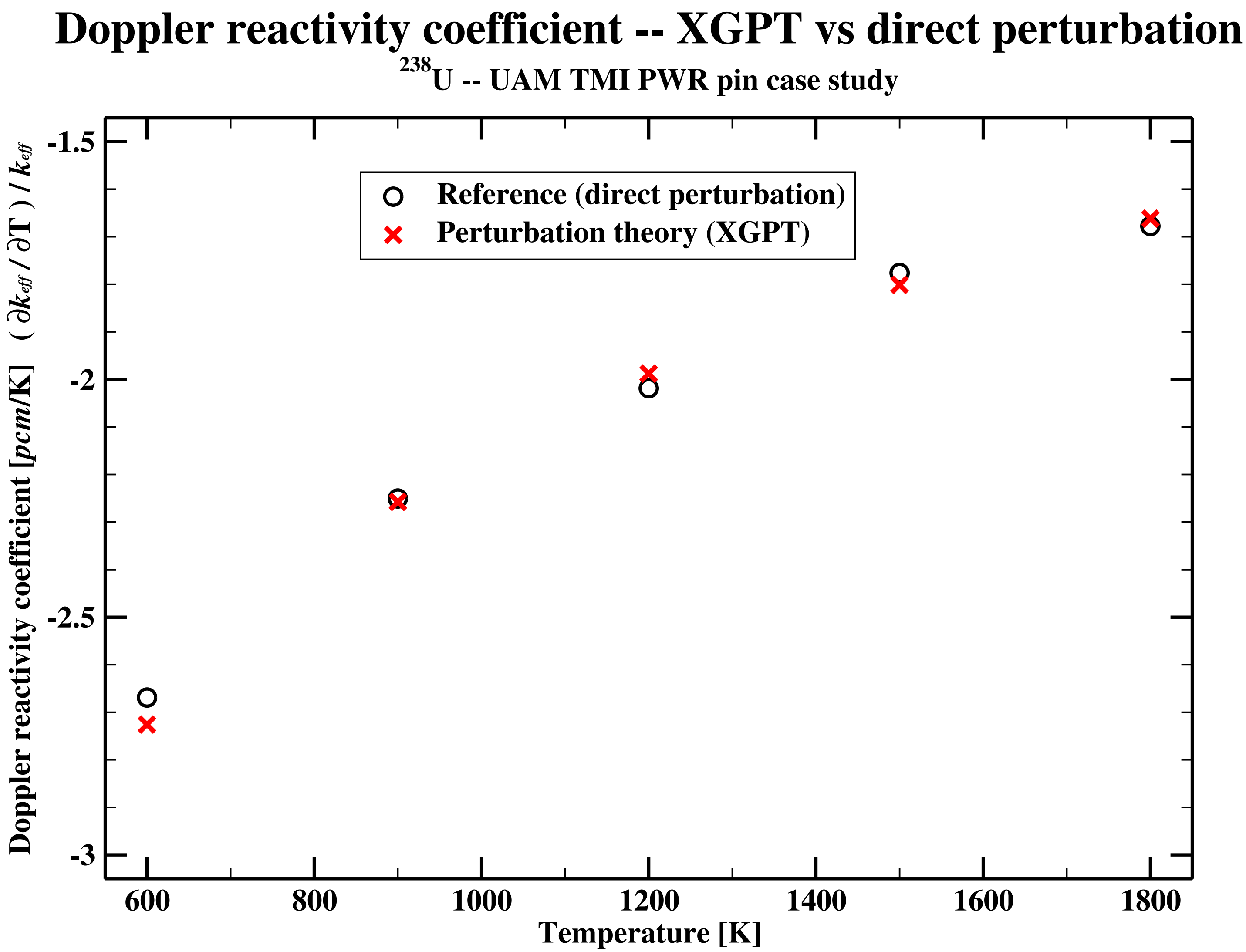


Different applications of xGPT capabilities

Questions? Suggestions?
Ideas?

Projection vs. discretization

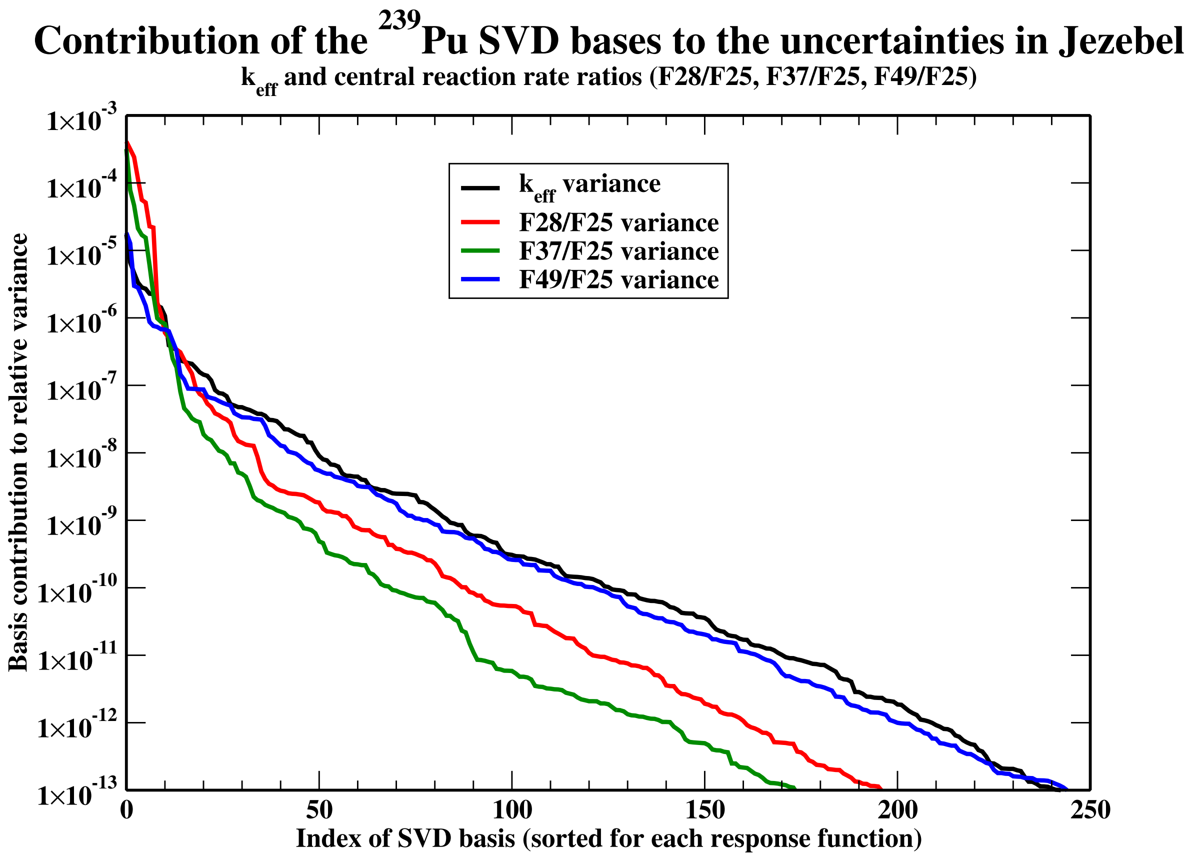


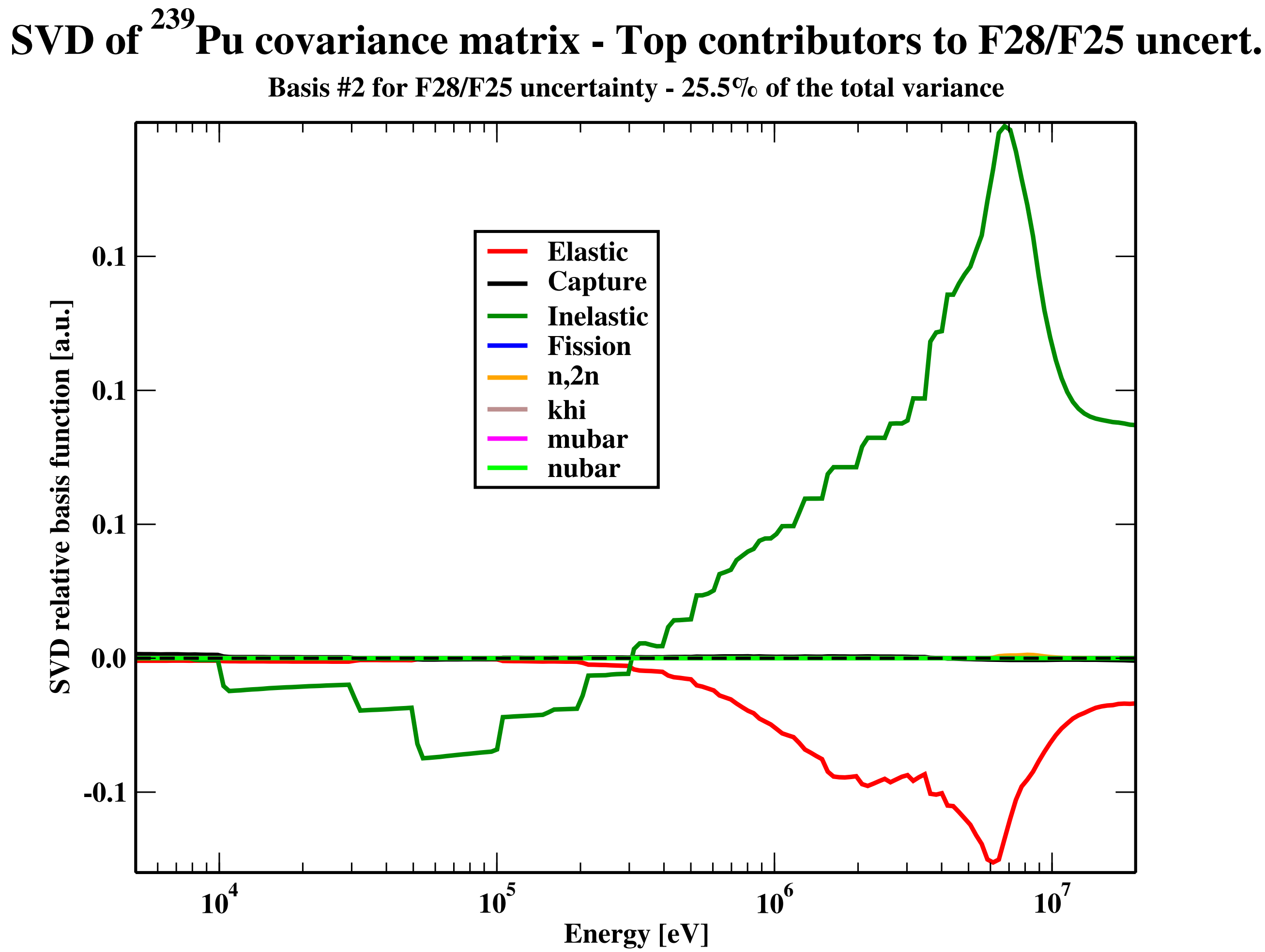
Figure: Eigenfunctions contribution to the total variances in Jezebel. Response functions: k_{eff} , F28/F25, F37/F25, F49/F25. (^{239}Pu ENDF/B-VII covariances).

Projection vs. discretization

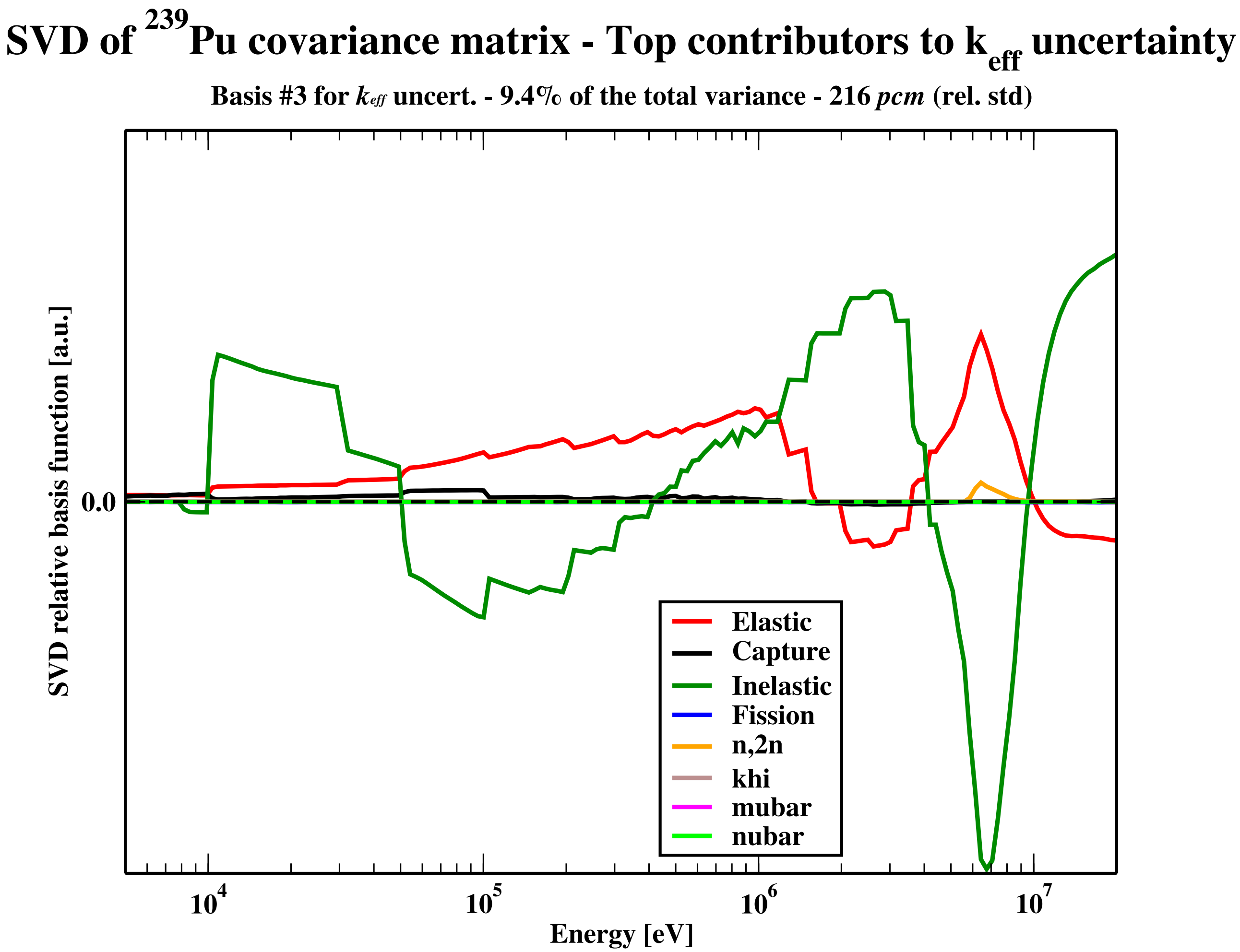
- Eigenvalue decomposition lead to exponential convergence with respect to the number of the basis functions
- Multi-group discretization lead to slow, unpredictable convergence with respect to the number of groups

- Statistical efficiency of Monte Carlo continuous sensitivity estimators doesn't depend on the number of eigenfunctions
- Statistical efficiency of Monte Carlo multi-group sensitivity estimators degrades quickly when adopting finer energy grids

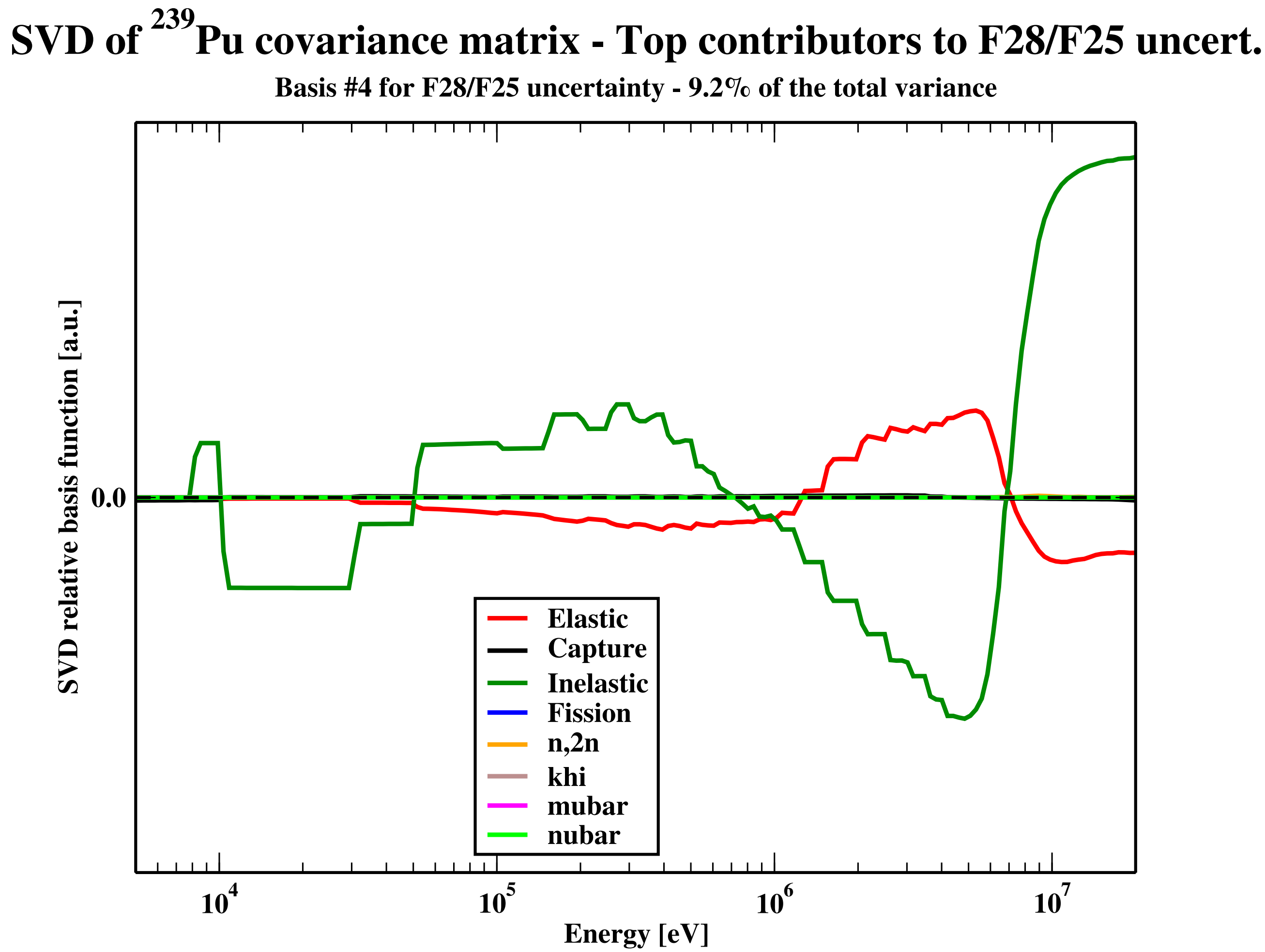
Example of basis functions from ^{239}Pu ENDF/B-VII



Example of basis functions from ^{239}Pu ENDF/B-VII



Example of basis functions from ^{239}Pu ENDF/B-VII



Multi-group/GPT starting point

Multi-group sensitivity coefficients:

$$\boldsymbol{S}_{\boldsymbol{\Sigma}}^{\boldsymbol{R}} = \left(S_{\Sigma_1}^{R}, S_{\Sigma_2}^{R} \cdots S_{\Sigma_N}^{R}\right) \tag{6}$$

Prior multi-group covariance matrices:

$$\boldsymbol{COV}\left[\boldsymbol{\Sigma}\,,\boldsymbol{\Sigma}\right] = \begin{bmatrix} Var(\Sigma_1) & COV\left[\Sigma_1\,,\Sigma_2\right] & \cdots & COV\left[\Sigma_1\,,\Sigma_N\right] \\ COV\left[\Sigma_2\,,\Sigma_1\right] & Var(\Sigma_2) & \cdots & COV\left[\Sigma_2\,,\Sigma_N\right] \\ \vdots & \vdots & \ddots & \vdots \\ COV\left[\Sigma_N 1\,,\Sigma_1\right] & COV\left[\Sigma_N\,,\Sigma_1\right] & \cdots & Var(\Sigma_N) \end{bmatrix} \tag{7}$$

Continuous-energy/XGPT starting point

Eigenfunctions sensitivities:

$$\mathbf{S}_{\mathbf{U}}^{\mathbf{R}} = \left(S_{U_1}^{R}, S_{U_2}^{R} \cdots S_{U_n}^{R}\right) \tag{8}$$

Projection of the (prior) covariance matrices:

$$\mathbf{COV}\left[\mathbf{U}\ ,\mathbf{U}\right] = \begin{bmatrix} V_1 & 0 & \cdots & 0 \\ 0 & V_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & V_n \end{bmatrix} \tag{9}$$

Adjusted continuous energy covariance

${}^{adjusted}\mathbf{COV}\,[\mathbf{U}\;,\mathbf{U}]$ via the Generalized Least Squares Method is obtained as:

$$
\begin{aligned}
&{}^{adjusted}\mathbf{COV}\,[\mathbf{U}\;,\mathbf{U}] - {}^{prior}\mathbf{COV}\,[\mathbf{U}\;,\mathbf{U}] = \\
&= \mathbf{M}\,\mathbf{G}^{T}\left[\mathbf{G}\,\mathbf{M}\,\mathbf{G}^{T} + \mathbf{V_e} + \mathbf{V_m}\right]^{-1}\,\mathbf{G}\,\mathbf{M}
\end{aligned}
\tag{10}
$$

${}^{adjusted}\mathbf{COV}\,[\mathbf{U}\;,\mathbf{U}]$ contains the correlations among the basis functions introduced by the experiments.

$$
\begin{aligned}
&{}^{adjusted}COV\left[\Sigma(E)\;,\Sigma(E')\right] \simeq \\
&\simeq \left[U_1(E) \quad \dots \quad U_n(E)\right]\;{}^{adjusted}\mathbf{COV}\,[\mathbf{U}\;,\mathbf{U}]\begin{bmatrix} U_1(E') \\ \vdots \\ U_n(E') \end{bmatrix}
\end{aligned}
\tag{11}
$$

Case study: Jezebel ^{239}Pu

Relative experimental uncertainties

k_{eff}	F28/F25	F37/F25	F49/F25
0.002	0.011	0.014	0.009

Experimental correlation matrix

	k_{eff}	F28/F25	F37/F25	F49/F25
k_{eff}	1.00	0.00	0.00	0.00
F28/F25	0.00	1.00	0.32	0.23
F37/F25	0.00	0.32	1.00	0.23
F49/F25	0.00	0.23	0.23	1.00

Table: Experimental uncertainties and correlation matrix for the four considered response functions.

Case study: Jezebel ^{239}Pu

Relative modeling uncertainties

k_{eff}	F28/F25	F37/F25	F49/F25
0.0018	0.0090	0.0030	0.0030

Modeling correlation matrix

	k_{eff}	F28/F25	F37/F25	F49/F25
k_{eff}	1.00	0.00	0.00	0.00
F28/F25	0.00	1.00	0.50	0.50
F37/F25	0.00	0.50	1.00	0.50
F49/F25	0.00	0.50	0.50	1.00

Table: Modeling uncertainties and correlation matrix for the four considered response functions.

Case study: Jezebel ^{239}Pu

	Exp.	Calc. (this work)	Calc. (WPEC-SG33)
k_{eff}	1.0000	0.99976	0.99986
F28/F25	0.2133	0.20871	0.20839
F37/F25	0.9835	0.97155	0.97071
F49/F25	1.4609	1.42435	1.42482

Table: Experimental and calculated values.

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Negative correlations

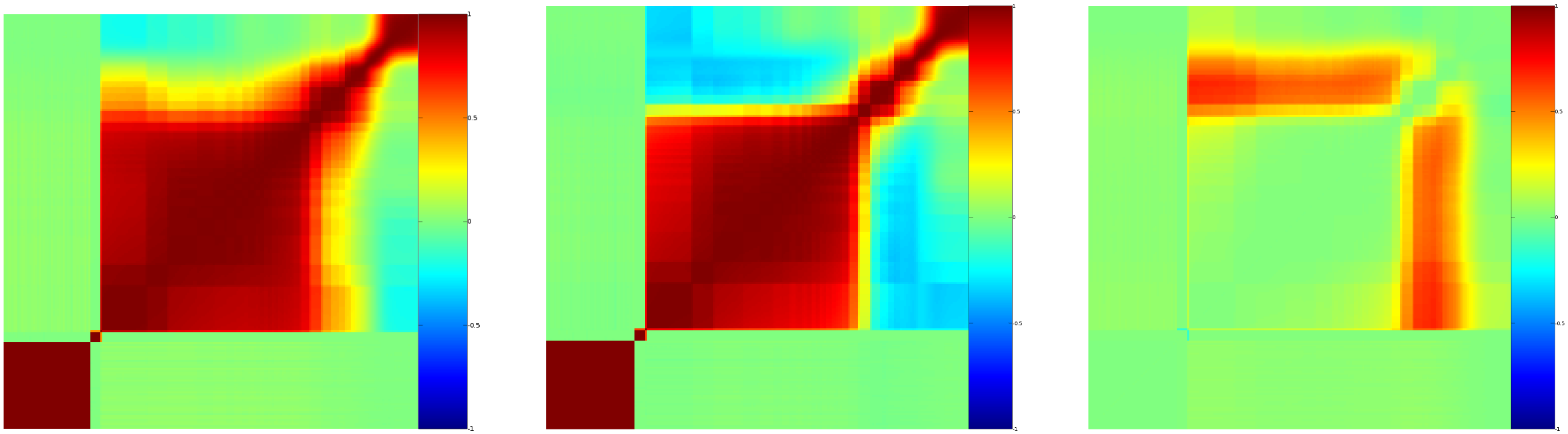

Figure: ^{239}Pu inelastic scattering correlation matrix in the 1 keV – 20 MeV energy region. Before (left) and after (center) the continuous energy adjustment process, and Prior – Post difference is shown on the right.

Conclusions

Main goal: new methodology for continous-energy XS adjustment

Shorten the distance between evaluators and Monte Carlo users (?)

Enable the adoption of integral experiments in a simple, effective and timely way (^{35}Cl (n, p), ^{233}U (n, γ)...)

Conclusions

Main goal: new methodology for continous-energy XS adjustment

Shorten the distance between evaluators and Monte Carlo users (?)

Enable the adoption of integral experiments in a simple, effective and timely way (^{35}Cl (n, p), ^{233}U (n, γ)...)

First tests are promising... we need to move to broader case studies. **Anyone wants to help/contribute???**

In the resonance region, resonance parameters XS sensitivities (after MF-32 decompositions) and scattering radii are the basis functions for the continuous adjustment

Lessons learned (random thoughts) and ongoing works

- Please, leave MF-32 in the ENDF files
- In the future, storing MF-33 in the form of eigenvectors/eigenvalues might save, memory, CPU, and headaches
- Now working on secondaries distribution adjustment... Legendre or double differential?
- Next step: URR adjustment (this might take some time!)